A homogenized model for porous single crystals containing general ellipsoidal voids

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Résumé : (16 gras)

Le but de cette étude est de proposer un modèle d'endommagement ductile viscoplastic pour les matériaux monocristallins à anisotropie cristalline arbitraire (FCC, BCC, HCP etc). Le modèle développé, appelé modèle variationel modifié (MVAR), est basé sur une méthode d'homogénéisation non linéaire qui utilise un composite linéaire de comparaison. Des simulations éléments finis multipores périodiques ont ensuite été effectuées dans l'optique de valider le modèle MVAR pour une large gamme de paramètres incluant l'anisotropie cristalline, différents exposants de fluage, plusieurs triaxialités de contraintes, angle de Lode, différents niveaux de porosité et de multiples formes ellipsoidales de pores (ratios d'aspect). Les premiers résultats obtenus se révelent très prometteurs.

Abstract : (16 gras)

The goal of the present study is to propose a viscoplastic constitutive model for porous single crystals with arbitrary crystal anisotropy (e.g., FCC, BCC, HCP etc). The proposed model, denoted as modified variational model (MVAR), is based on the nonlinear variational homogenization method, which makes use of a linear comparison porous material to estimate the response of the nonlinear porous single crystal. Periodic multi-void finite element simulations are used in order to validate the MVAR for a large number of parameters including cubic (FCC, BCC) and hexagonal (HCP) crystal anisotropy, various creep exponents (i.e., nonlinearity), several stress triaxiality ratios, general void shapes and orientations and various porosity levels. The first results seem to be very promising.

Crystal plasticity, Porous materials, Homogenization

1 Introduction (16 gras)

Voids originate in the manufacturing process have an important effect on the lifetime of materials and play a important role even on metallic alloys. Indeed, as recently indicated by experimental observations ([1]) at high enough temperatures on tensile specimens, the growth of initially present processing induced voids in a nickel based single crystal superalloy as well as in standard polycrystals played a significant role in limiting creep life. The presence of voids in metals is known to be one of the major causes of ductile failure, as addressed in pioneering works by ([2,3,4]). Most of the studies have been carried out in the case of two-phase material systems comprising an isotropic rate independent matrix phase (metal usually described by von Mises yield criterion) and a voided phase (pores of spherical, spheroidal or arbitrary ellipsoidal shapes).

Far fewer results have been obtained for rate-dependent anisotropic matrix systems, generally based on a phenomenological Hill-type matrix. However, there is no damage ductile growth model for the case of porous single crystals. When these material systems are subjected to external loads impurities fail or decohere leading to the creation of pores, which in turn evolve in size, shape and orientation ([5]). This complex evolution of microstructure together with the evolution of the rate-dependant matrix anisotropy is critical in the prediction of the eventual fracture of the specimen under monotonic and cyclic loading conditions.

The purpose of the present work is to develop a model to deal with rate-dependent crystalline matrix phase comprising general ellipsoidal voids that could possibly evolve in shape and orientation, using a variational homogenization framework. The prediction capabilities of the model are compared with finite element computations obtained from unitary and multiple void unit-cells.

2 Results and discussion

The numerical validation of the model has been carried out through FEM, with periodic geometry (see fig 1).

As an important result depicted in fig 2, the present estimate takes into account the anisotropy of the single crystal and the anisotropy of the microstructure. Moreover, the MVAR model has been able to predict the strong dependence of the effective response, and especially of the average hydrostatic stress upon the number and orientation of the slip systems as well as the shape and orientation of the voids. One of the major finding of this work, is that for highly anisotropic crystals (e.g., three basal active slip systems in certain HCP crystal structure) the porous crystal can exhibit fully incompressible response, even in the presence of voids. This of course affects the entire effective response of the porous crystal for the entire range of stress states. That is the first time such a result is presented in the literature and reveals the significance of plastic anisotropy of the underlying phases upon the macroscopic response of the material.

Furthermore, it has been shown that the void shape and orientation affect strongly the response of the porous crystal. In particular, the effective response becomes much

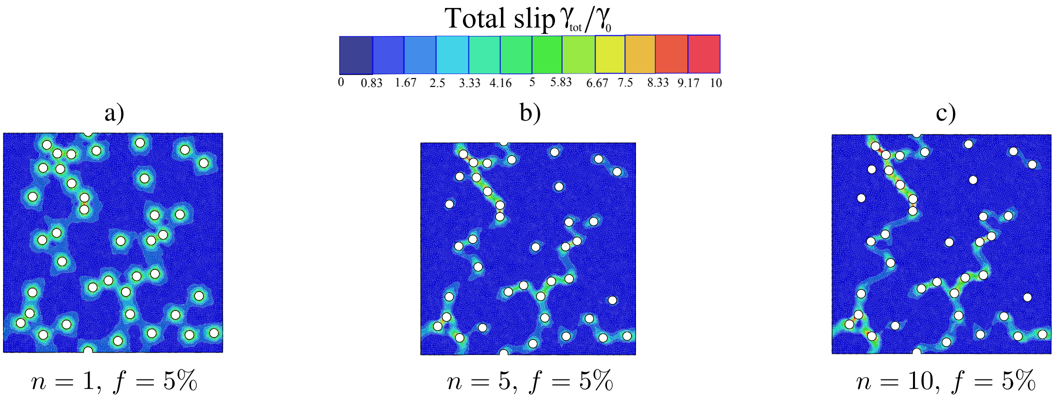

Figure 1: Contour of the total slip for a FCC single crystal with a "multipore" geometry of 40 pores (porosity $f = 5\%$), and several creep exponent (a) $n = 1$ (b) $n = 5$ (c) $n = 10$.

softer as one goes from a spherical void to an ellipsoidal one (which is suggestive of a crack-type geometry). In the general case of ellipsoidal voids arbitrarily oriented (with respect to the laboratory axes) and arbitrary crystallographic texture, we have shown that the effective response exhibits no symmetries when plotted in a purely deviatoric plane (and at finite hydrostatic stresses) thus indicating the non-trivial coupling between the anisotropy of the underlying crystal and the (morphological) anisotropy induced by the shape and orientation of the voids.

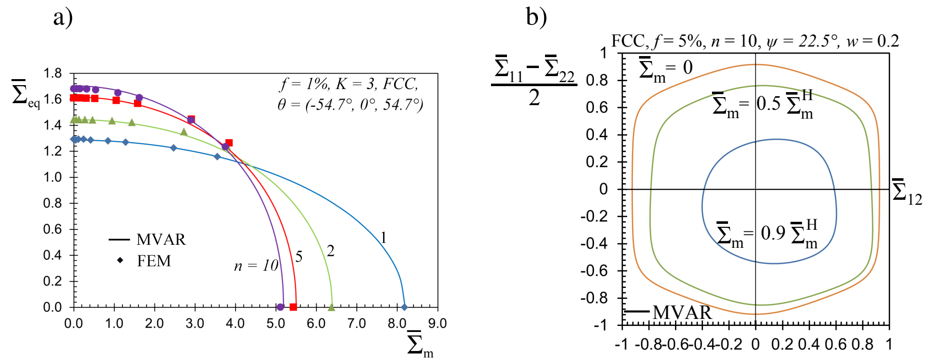

Figure 2: Gauge surface for a porous FCC crystal with elliptical voids. (a) Comparison between the model (MVAR) and the FE results in the $\overline{\Sigma}_m - \overline{\Sigma}_{eq}$ plane, for a porosity $f = 1\%$ and a range of creep exponent $n = (1, 2, 5, 10)$. (b) In the deviatoric plane $\overline{\Sigma}_{12} - - \left(\overline{\Sigma}_{11} - \overline{\Sigma}_{22}\right)/2$ for a creep exponent $n = 10$, voids of aspect ratio $w = 0.2$, orientation $\psi = 67.5^o$, a porosity $f = 5\%$, at different level of pressure.

Références

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